[Teaching Points for PyMol 3 Lab](http://vdsclass.wordpress.com/?p=1796" \o "Teaching Points for PyMol 3 Lab)

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Students should be getting into a groove with PyMol now. So, this one shouldn’t be too hectic. Also, they don’t have a lab report due for this one.  **BUT** – there notebook must be well done and they will have to put some ANALYSIS in their notebook.

**IMPORTANT CONCEPTS:**

Reinforce the concept that primary sequence doesn’t have to match for two enzymes to have similar function (just the active sites need to be similar enough).

**IMPORTANT SKILLS:**

* creating an active site using the line commands
* Being able to define binding interactions (H-bond, salt bridges, hydrophobic interactions) for a ligand and make a subjective comparison of binding.
* Understanding that van der Waals contacts are not shown in PyMol – but rather they are still important to ligand binding because they are ‘all over the place’

Note: A lot of stuff has been changed in this lab from last year.

They will have 2 different proteins loaded at the same time. So, in order to prevent PyMol from creating cross bonds between the *Lactobacillus*molecules and the *Homo sapiens* molecules, they will need to make a selection that is a **COMPLEX** of *Lactobacillus* protein and the NADPH with the Lactobacillus Active Site. And the same thing for the human Active site:

If they start showing bonds going to the atoms of the different species or going ‘off into space’ – they probably didn’t do it right.

Make sure they save their files often (preferably naming session files with different names every once in a while) so that they can go back if they mess something up.

Force them to save their files to an ONLINE location for storage (UT Webpsace)

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